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Abstract

We test an isospectral potential from harmonic oscillator simulating H-bond interaction in DNA macromolecules.

1 Introduction

In the context of Supersymmetric Quantum Mechanics (SQM), several new potentials have been generated from shape invariant potentials[1] . In particular, with reference to the harmonic oscillator[2-4]. However, to date, none of these new potentials have been applied to real physical systems.

Peyrard and Bishop[5] have introduced a theoretical treatment of DNA. In this model, starting from the classical Hamiltonian and using the transfer integral operator, the partition functions follow from the eigenvalues of a Schrödinger-type equation.

We intend, in this communication, to demonstrate the feasibility of using a new potential generated from the harmonic oscillator in the Schrödinger-type equation to describe H-bonds in DNA.

2 SQM

In SQM the nilpotent operators Q and Q^+ satisfy the algebra[6]

$$\{Q, Q^+\} = H_{SS}; Q^2 = Q^{+2} = 0 \quad (1)$$

which can be realized in a usual matrix form. In this case, the supersymmetric Hamiltonian H_{SS} consists of two partners H_+ and H_- which can be factorized in $H_+ = a^+ a^-$ and $H_- = a^- a^+$ (where a^\pm bosonic operators), and they have the same spectra except for the ground state, where only H_+ has an eigenvalue equal to zero $E_+ = 0$. The eigenfunctions of H_+ and H_- are related to one another by: $\Psi_+ = a^+ \Psi_-$ and $\Psi_- = a^- \Psi_+$, where the bosonic operators are defined by:

$$a^\pm = \left\{ \mp \frac{d}{dx} + W(x) \right\}. \quad (2)$$

Redefining the operators a^\pm , it is possible to obtain a family of Hamiltonians as shown by Sukumar[7], or the isospectral potentials[2-4]. In this second case defining new operators:

$$A^\pm = \mp \frac{d}{dx} + F(x) \quad (3)$$

and imposing $H_- = A^- A^+$ yields a general form to get $F(x)$. The new Hamiltonian is written as

$$\tilde{H}_+ = A^- A^+ - 2 \frac{d}{dx} F(x) \quad (4)$$

and the eigenfunctions of the new Hamiltonian are related to the original Hamiltonian ones. The missing ground state is obtained from $A^- \Psi_{+,0} = 0$.

As an example, consider the original potential to be the harmonic oscillator, $V(x)=x^2$. It then follows[1-4] :

$$\tilde{H}_+ = -\frac{d^2}{dx^2} + x^2 - 1 - 2 \frac{d}{dx} \frac{\exp(-x^2)}{\Gamma_+ \int_0^x \exp(-z^2) dz} \quad (5)$$

$$\Psi_{+,0} = \exp\left\{-x^2 + \int_0^x \frac{\exp(-z^2) dz}{\Gamma_+ \int_0^z \exp(-y^2) dy}\right\}. \quad (6)$$

3 DNA Model

Bishop & Peyrard's DNA model includes two degrees of freedom (u_n, v_n) corresponding to displacements of the bases from their equilibrium positions along the direction of the H-bonds connecting them. A harmonic coupling due to the stacking interactions between neighboring bases is also assumed with the same coupling constant (k) for the two strands. Each base has the mass m .

The Hamiltonian for this model is

$$H = \sum_n \left\{ \frac{p_n^2}{2m} + \frac{k}{2} (x_n - x_{n-1})^2 + \frac{q_n^2}{2m} + \frac{k}{2} (y_n - y_{n-1})^2 + V(y_n) \right\}, \quad (7)$$

where $x_n = (u_n + v_n)/\sqrt{2}$, $y_n = (u_n - v_n)/\sqrt{2}$, $p_n = m\dot{x}_n$, $q_n = m\dot{y}_n$ and $V(y_n)$ is the potential for the hydrogen bonds. Using the transfer integral operators to solve configuration integral energy the classical partition function can be obtained.

The temperature of denaturation of DNA can be monitored through the mean stretching $\langle y_n \rangle$ of the H-bond. Considering the limit of large N , only the ground state will be important, and

$$\langle y \rangle = \langle \Phi_0(y) | y | \Phi_0(y) \rangle = \int \Phi_0^2(y) y dy, \quad (8)$$

where $\Phi_0(y)$ is the ground state eigenfunction of a Schrödinger-type equation:

$$\left\{ -\frac{1}{2\beta^2 k} \frac{d^2}{dy^2} + V(y) \right\} \Phi_i(y) = \left\{ \epsilon_i + \frac{1}{2\beta} \ln \frac{2\pi}{\beta k} \right\} \Phi_i(y). \quad (9)$$

It is important to note the mean value $\langle y \rangle$ depends on the form of the eigenfunction $\Phi_0(y)$.

4 H-bond Potential

The Morse potential is usually used to simulate the H-bonds in DNA. However, we suggest here that the potential generated from the harmonic oscillator using the superalgebra can also be used. This potential has the form:

which can be realized in a usual matrix form. In this case, the supersymmetric Hamiltonian H_{SS} consists of two partners H_+ and H_- which can be factorized in $H_+ = a^+ a^-$ and $H_- = a^- a^+$ (where a^+ and a^- are bosonic operators), and they have the same spectra except for the ground state, where only H_+ has an eigenvalue equal to zero $E_+ = 0$. The eigenfunctions of H_+ and H_- are related to one another by: $\Psi_+ = a^+ \Psi_-$ and $\Psi_- = a^- \Psi_+$, where the bosonic operators are defined by:

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$$\Psi_{+,0} = \exp \left\{ -x^2 + \int_0^x \frac{\exp(-z^2) dz}{\Gamma + \int_0^z \exp(-y^2) dy} \right\}. \quad (6)$$

3 DNA Model

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